E-K Diagram, and Brillouin Zones

Topics to be covered

:

- Preliminary ideas of Kronig Penney Model
- Introduction
- E-K diagram
- Brillouin zones in one dimension zones
- References

Objectives

- Explain and apply E-K Diagram
- Explain Brillouin zones

Kronig-Penney Model

- For electron in a periodic potential it assumes that the potential energy of an electron forms a periodic square potentials of periods (a+b) such that

$$V(x) = V_0 \quad \text{for } -b < x < 0$$
$$= 0 \quad \text{for } 0 < x < a$$

- This model, although idealised but very useful because it explains many useful periodic features of the behaviour of electron-lattices.
- The wave functions associated with this model may be calculated by solving Schrodinger equations in two regions:

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\Psi = 0 \quad for\ 0 < x < a \text{..}(2a)$$

$$\frac{d^2\psi}{dx^2} + \frac{2m(E-V_0)}{\hbar^2}\Psi = 0 \quad for\ -b < x < 0 \text{...................................}(2b)$$

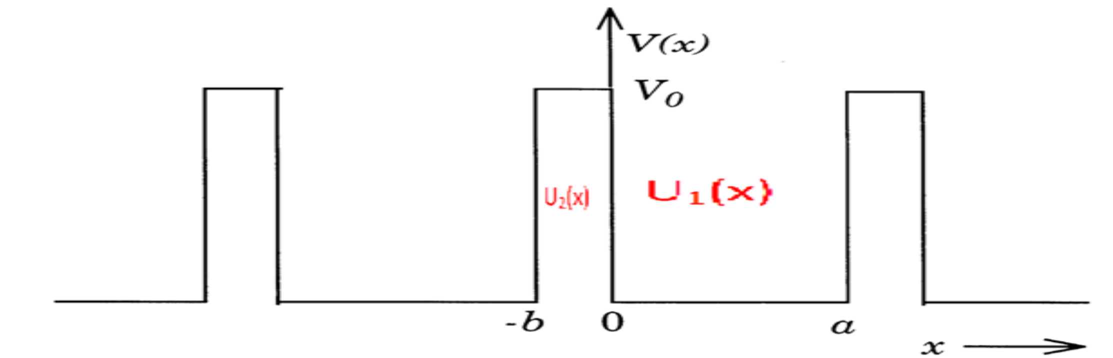


Fig. 2 Square well periodic potential as introduced by Kronig and Penney

$$\frac{2mE}{\hbar^2} = \alpha^2 \ and \ \frac{2m(V_0 - E)}{\hbar^2} = \beta^2 \text{.............................}(3)$$

$$\frac{d^2\psi}{dx^2} + \alpha^2\Psi = 0 \text{...}(4a)$$

$$\frac{d^2\psi}{dx^2} - \beta^2\Psi = 0 \text{..}(4b)$$

Prerequisite

Using boundary condition we can solve it to the condition for the solutions of the wave equation to exist

$$\frac{m V_0}{\alpha\beta \hbar^2}\beta b \sin \alpha a + \cos \alpha a \cong \cos ka$$

$$P\frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka \quad ----------------(7)$$

where P= $\frac{m V_0}{\hbar^2} a b$

P is a measure of the quantity $V_0 b$, which is the area of potential barrier, called barrier strength

If P is large the barriers are strong. When P→∞, corresponding to a infinitely deep potential well, the electron can be considered as confined into a single potential well. This case applies to crystals where the electrons are very tightly bound with their nuclei.

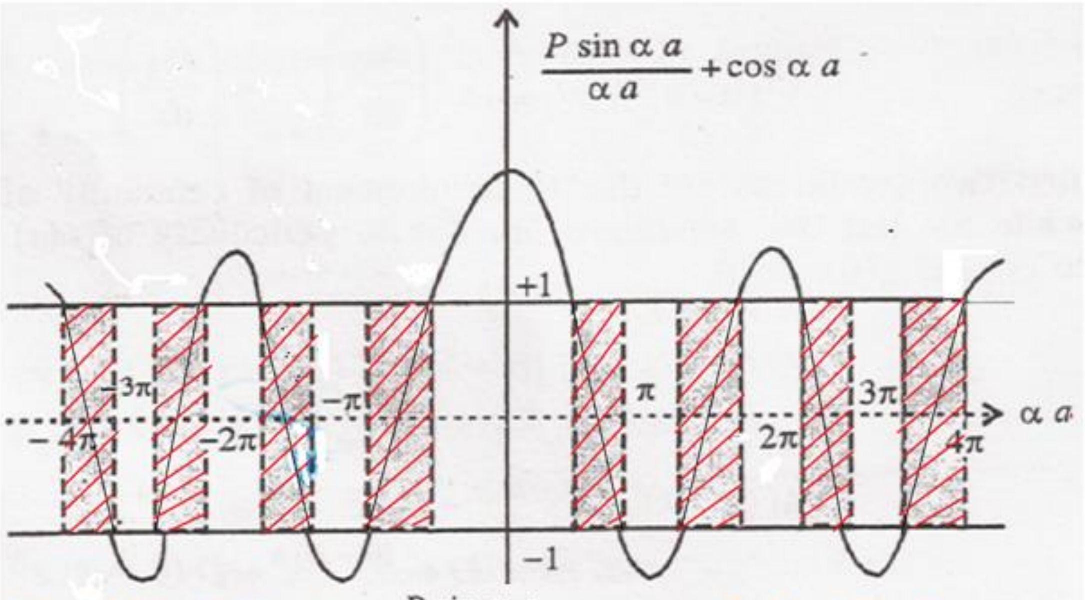


Fig.3: Plot the function $\left(\frac{P \sin \alpha a}{\alpha a} + \cos \alpha a\right)$ for P=3π/2 where allowed energy band is represented by the shaded region

Introduction

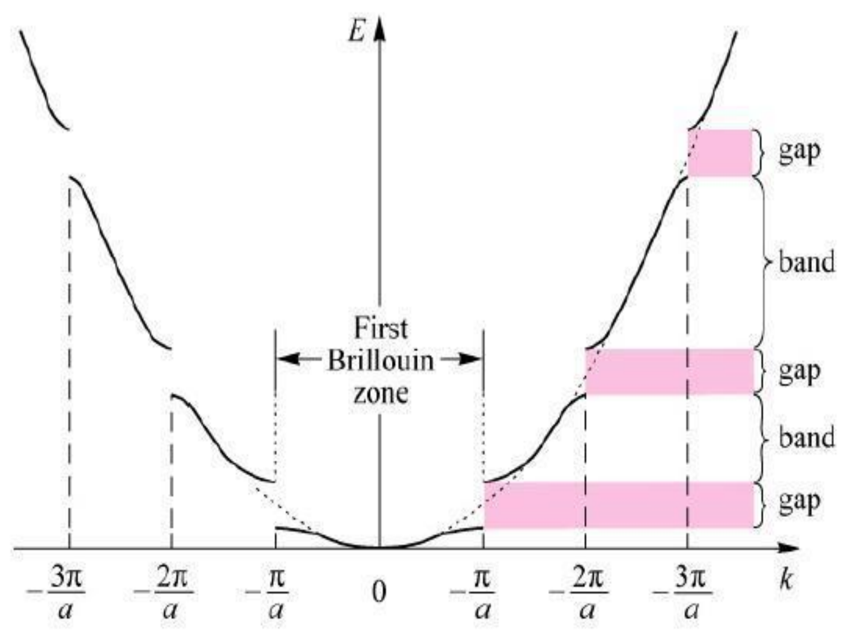
- An E-k diagram shows characteristics of a particular semiconductor material.
- It shows the relationship between the energy and momentum of available quantum mechanical states for electrons in the material.
- It gives the idea of band gap (E_G), the difference in energy between the top of the valence band and the bottom of the conduction band.

E-K Diagram

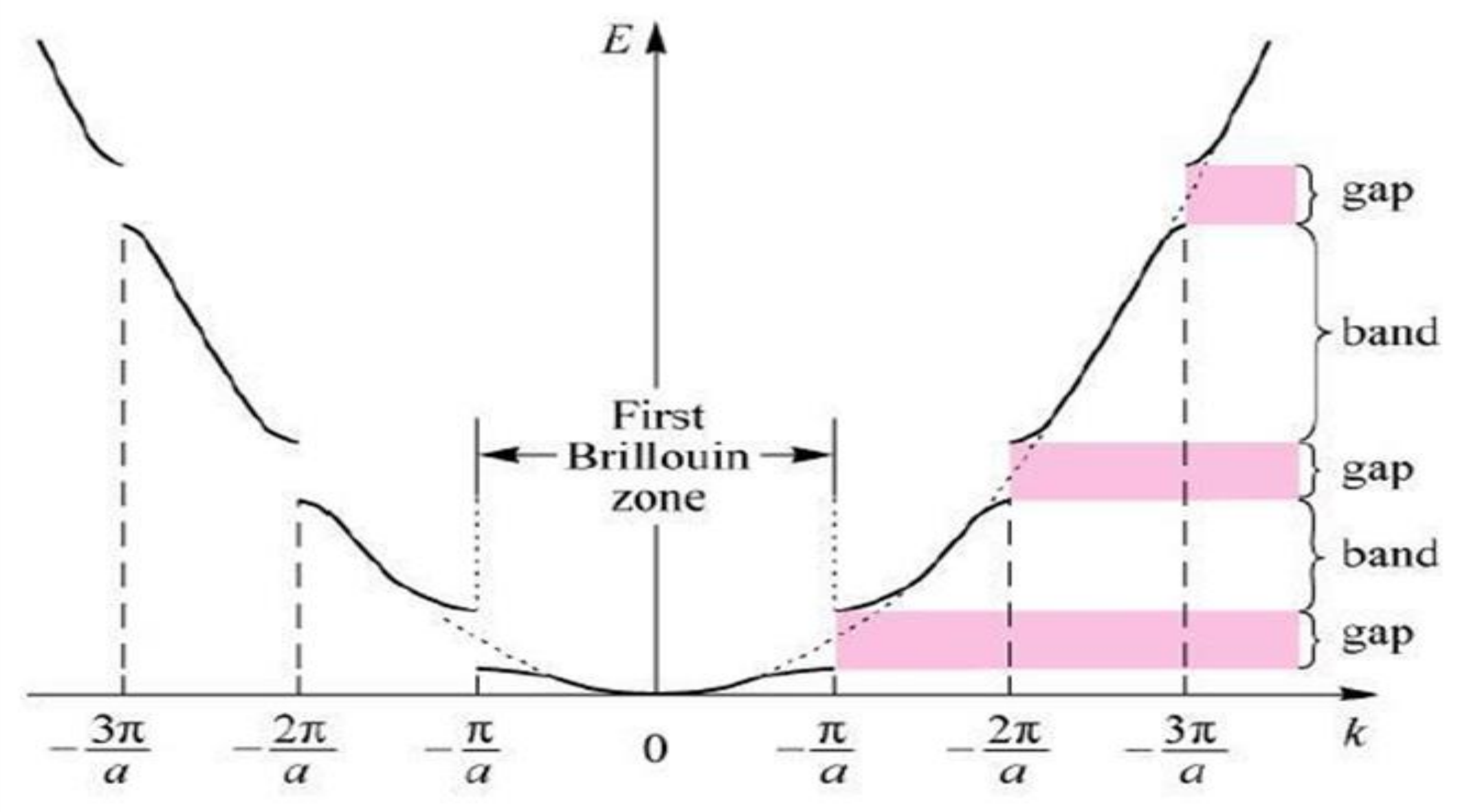
- The electron moving in a periodic potential lattice can have energy values only between allowed regions or zones. With the help of equation

$$P\frac{\sin\alpha a}{\alpha a} + \cos\alpha a = \cos ka \quad ------------------(1)$$

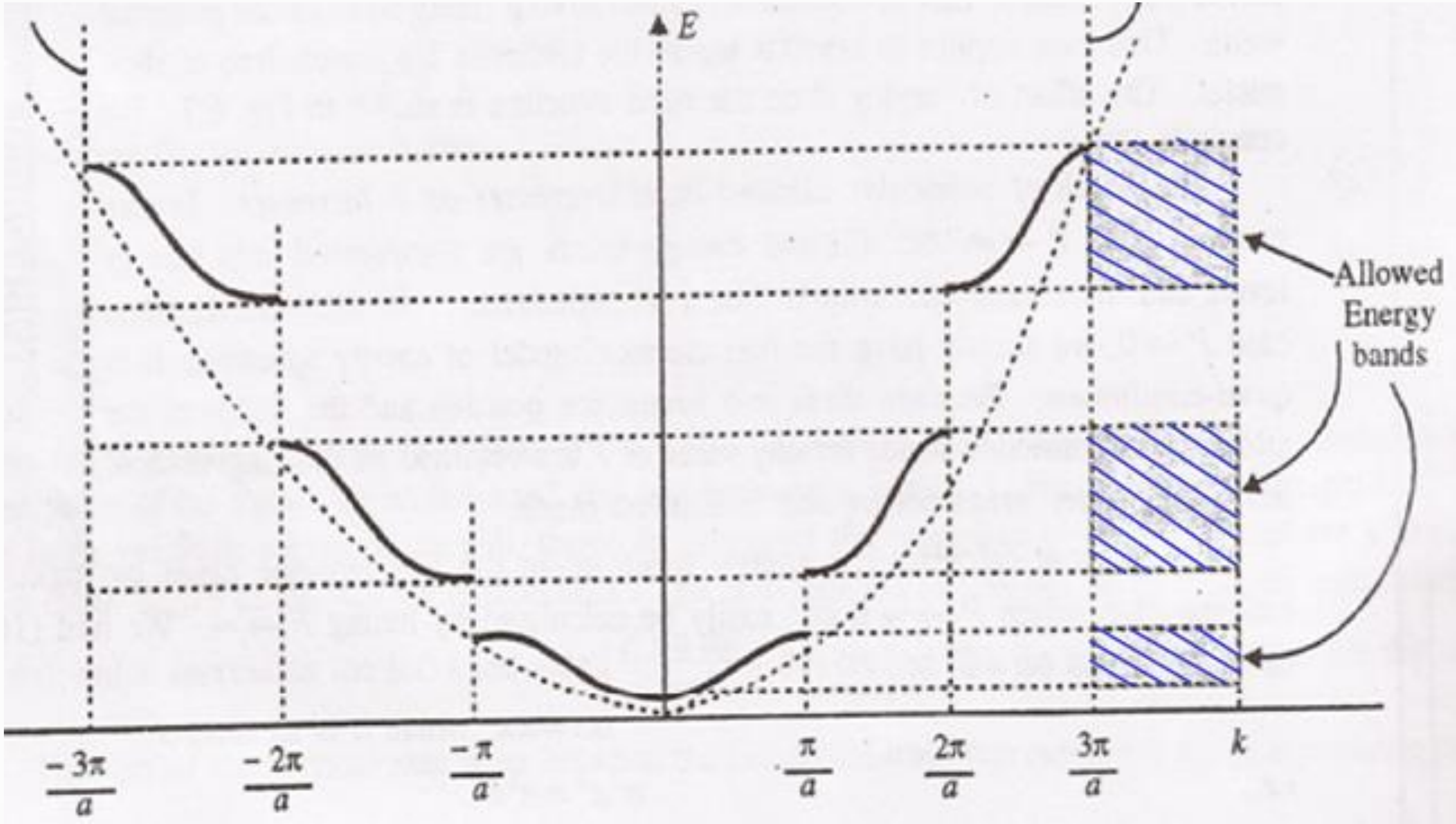
- The R. H.S. of the equation (1) cos ka becomes ±1 for values of k=nπ/a and hence the discontinuities in the E versus K graph occur at k=nπ/a where n takes the values of ±1, ±2, ±3, --- etc.
- The total energy E of the electron can be plotted versus the wave number, or the propagation vector 'K'



E-K Diagram

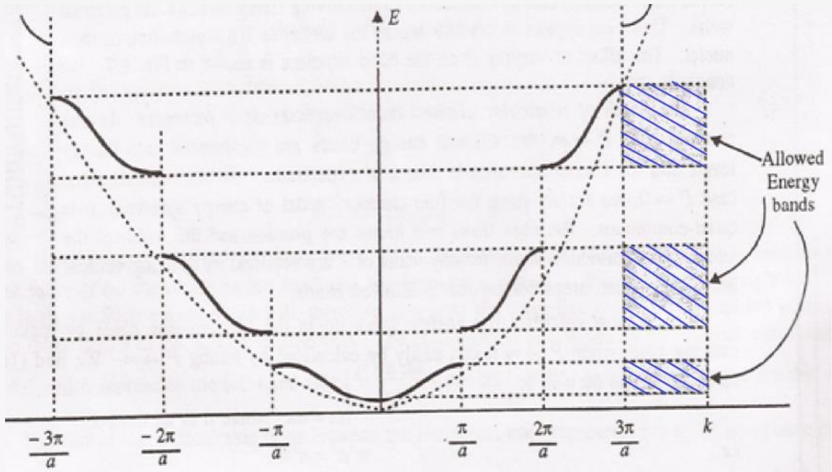


E
First
Brillouin
zone
gap
band
gap
band
gap
$-\frac{3\pi}{a}$
$-\frac{2\pi}{a}$
$-\frac{\pi}{a}$
0
$-\frac{\pi}{a}$
$-\frac{2\pi}{a}$
$-\frac{3\pi}{a}$
k


E
Allowed
Energy
bands
$\frac{-3\pi}{a}$
$\frac{-2\pi}{a}$
$\frac{-\pi}{a}$
$\frac{\pi}{a}$
$\frac{2\pi}{a}$
$\frac{3\pi}{a}$
k

E-K Diagram

- When $P \rightarrow 0$, corresponds to no barrier, the electron can be considered to be moving freely through the potential wells.



$\cos \alpha a = \cos ka$ i.e., $\alpha = k$ or $\alpha^2 = k^2$

$$\frac{2mE}{\hbar^2} = k^2$$

$$\frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}, \quad [As\ k = \frac{2\pi}{\lambda}, \lambda = \frac{h}{p}]$$

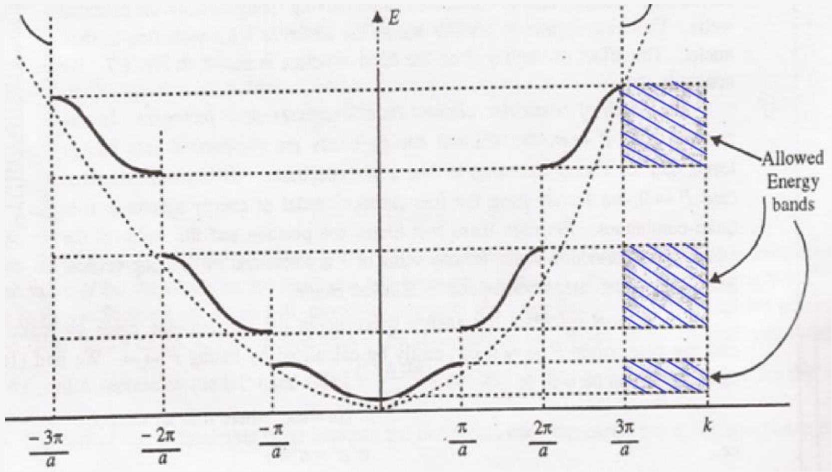
$$E = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m}, \quad [As\ k = \frac{2\pi}{\lambda}, \lambda = \frac{h}{p}]$$

which is appropriate to the completely free particle. This shows that the allowed energy states of electron are continuous

The dotted curve shows the parabola of free electron i.e.,

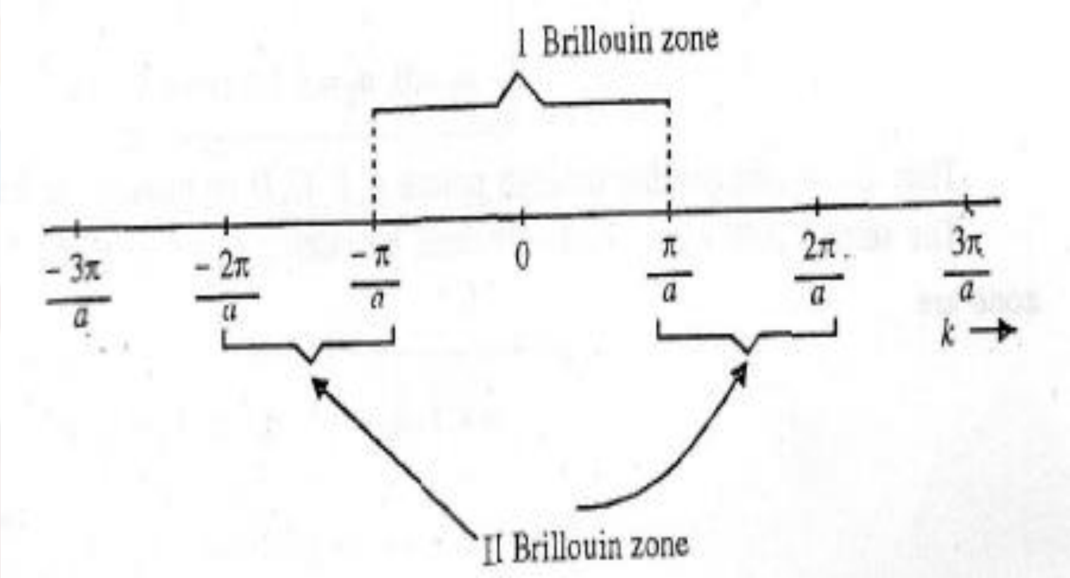
E-K Diagram

- In a periodic potential lattice, the electron energy values are discontinuous, separated into allowed and forbidden zones occurring alternatively.
- The width of the forbidden band increases with E.
- As P decreases, the discontinuous E-K graph will reduce to a continuous parabolic graph as shown by dotted lines and the forbidden bands disappear. This means that the energy values become practically continuous, when the perturbations of the potential due to periodicity of the lattice vanish, making electrons really free.



Brillouin zones in one dimension

In one dimensional periodic lattice, the energy discontinuities occur when the wave number k satisfies the condition k = nπ/a where n is a +ve or –ve integer. If we consider a line Fig 6, representing k values divided into energy discontinuities into segments of length ±π/a, then these line segments are known as Brillouin zones



The first segment $-\frac{\pi}{a} < k < +\frac{\pi}{a}$ is called the First Brillouin zone.

$-\frac{2\pi}{a} < k < -\frac{\pi}{a}$ *and* $k = \frac{\pi}{a}$ *to* $\frac{2\pi}{a}$, This zone is called second Brillouin zone

Practice Questions

1. Draw and explain E-K diagram.

2. Draw and explain Brillouin zones in one dimension

References

1. J. Singh , Semiconductor optoelectronics, Physics and Technology, Mc-Graw –Hill Inc. 1995.

2. S.M. Sze, Semiconductor Devices: Physics and Technology, Wiley 2008.

3. Pillai S O, Solid State Physics,(2010), sixth edition, New Age International (P) Ltd. ISBN-9788122427264.